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AIR QUALITY ASSESSMENT MODEL (AQAM)
VERIFICATION ANALYSIS

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PREFACE

The Computer Outputs listed below will be maintained at the USAFOEHL Library on microfiche. They are lengthy and difficult to reproduce for the report. The computer outputs of each model as it existed in 1976, 1984 and 1986 can be easily compared. For each version, a listing of user supplied data, source inventory, and short term dispersion is included.

- A-1, User Supplied Data Processed by AQAM-76
- A-2, User Supplied Data Processed by AQAM-84
- A-3, Reformatted Data Processed by AQAM-86
- B-1, Source Inventory Listing AQAM-76
- B-2, Source Inventory Listing AQAM-84
- B-3, Source Inventory Listing AQAM-86
- C-1, Short Term Dispersion Listing AQAM-76
- C-2, Short Term Dispersion Listing AQAM-86

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1.0 INTRODUCTION

The United States Air Force Occupational and Environmental Health Laboratory (USAFOEHL) contracted with the Research Triangle Institute (RTI) to upgrade the Air Quality Assessment Model (AQAM), a computer-based numerical model for assessing air base source emissions and for predicting the dispersion of pollutants in the atmosphere (see Ref. 1).

The AQAM system, created in 1976, was transferred in 1983 to operational status at USAFOEHL (see Ref. 2). The acquisition by USAFOEHL in 1984 of a Digital Equipment Corporation VAX-11/780 computer offered (1) a more convenient host for AQAM and (2) the opportunity for enhancing the model with a user-friendly operating interface and graphical-output options.

To verify the performance of AQAM on its new host, RTI was required to repeat an air-quality analysis for Williams AFB that was first performed in 1976 as part of the AQAM verification process. This report summarizes the results of this effort and documents that the AQAM system currently hosted on the USAFOEHL VAX-11/780 produces output which generally replicates that of the previous AQAM systems.

2.0 DISCUSSION

Because of the combined effect of several factors, it is difficult to reproduce with the new AQAM system the output of earlier AQAM systems. In order of importance, these factors are:

- o The lack of a reference version of the model to serve as a basis of comparison;
- o Changes in the reference data used by the model;
- o Errors in input data to the model;
- o Different computer hosts for the model.

The discussion which follows shows that the performance of the current model is at least consistent with that of the previous models and that any differences observed are attributable to one or more of the listed factors.

2.1 Procedure

The current version of AQAM, referred to here as AQAM-86, was used to process source data for Williams AFB. This set of data is probably the most extensive ever collected for an AQAM analysis, since it formed the basis for an experimental assessment of AQAM accuracy. The performance of AQAM-86 on these data was compared with that of two earlier versions of AQAM:

- o AQAM as it existed circa 1976 (AQAM-76);
- o AQAM as it existed when the current effort began in 1985 (AQAM-84).

Using AQAM-76 as a reference is appealing since this version of the system was involved in the experimental assessment program and is the only version of the model for which a good short-term dispersion analysis is available. Using AQAM-84, on the other hand, is desirable because it includes revised algorithms for computing aircraft takeoff-roll distances and ground service equipment (GSE) emissions. Complicating the issue are undocumented changes made to the model in the period between 1976 and 1984 that prevent AQAM-84 from duplicating AQAM-76. For example, divide-by-zero errors occur with AQAM-84.

2.2 Comparison of Source Input Data

Computer Output A contains listings of three versions of the Williams AFB source input data:

- o the user-supplied data processed by AQAM-76;
- o the user-supplied data processed by AQAM-84; and
- o the reformatted data processed by AQAM-86 (which appear only as intermediate data in the new AQAM and are, therefore, of limited interest to the AQAM user).

Note that the new data-entry procedures of AQAM-86 preclude a direct comparison of its input with those of earlier models. The reformatted source data of AQAM-86, however, should generally duplicate the user-supplied source data of the earlier AQAM versions.

Comparison of the three sets of input data shows several minor, but expected, deviations:

- o Datasets 2 and 11 are empty in AQAM-86 data since these data now enter the model as "Reference Data;"
- o Generally speaking, default values appear explicitly in AQAM-86 data, whereas they may appear as "blank fields" in AQAM-76 and AQAM-84 data;
- o Variations in Dataset 4 arise from inconsistent data used with AQAM-76 and AQAM-84 in counting aircraft arrivals and departures;
- o Datasets 8 and 10 show the change in format implemented in AQAM-86 to allow 24 aircraft to be processed;
- o Dataset 9 shows the effect of changing the GSE algorithm between 1976 and 1984 (see Ref. 3).

In all other respects, the three sets of input data are identical and should lead to similarly identical analysis results.

The subsections which follow discuss the source inventory output and the short-term dispersion output produced by the three versions of AQAM.

2.3 Comparison of Source Inventory Analyses

Computer Output B contains source inventory listings produced by AQAM-76, AQAM-84, and AQAM-86. Comparison of the three listings reveals the several differences enumerated below. Discussed is only the first appearance of a deviation between versions of AQAM; in most cases the effect of deviations will appear several times in listings, e.g., whenever summaries are computed.

- 2.3.1 Base descriptions and general comments. The list of air base sources produced by AQAM-86, a list which AQAM-84 for some reason chooses not to print, duplicates AQAM-76.
- 2.3.2 <u>Default Information (I.A.).</u> In AQAM-86, only information in the air base-specific reference database is printed; in AQAM-76 and AQAM-84, all information in the general AQAM reference database (as modified by Dataset 2) is printed.
- 2.3.3 Information on aircraft activity, parking areas, taxiways, and runways (I.B.1). The numbers of aircraft arrivals and departures listed by AQAM-86 differ from those of AQAM-84 because of the differences in arrivals and departures in Dataset 4 (see Sec. 2.2).
- 2.3.4 Aircraft emission factors by aircraft type (I.C.1). The runway roll emissions computed by AQAM-86 agree with those computed by AQAM-84 but differ from those computed by AQAM-76 because of a change in the algorithm which computes takeoff-roll distances (see Ref. 2).
- 2.3.5 Ground service equipment emissions (I.C.2). Differences among all three versions of AQAM occur in GSE emissions. Those between AQAM-86 and AQAM-84 are explained as in Section 2.3.3 above, since GSE emissions are dependent on aircraft activity. Those between AQAM-86 and AQAM-76 are caused by a change in the algorithm computing these emissions (see Ref. 3).
- 2.3.6 Air base power plants (II.B.4). The emissions for air base power plants computed by AQAM-86 show considerable deviation from those of AQAM-84 because of changes in "furnace" emission factors (changes which bring these factors into agreement with the latest version of AP-42 published by EPA). For comparison purposes, the factors appearing in these two versions of AQAM are shown in Figure 1.
- 2.3.7 Air base space heating (II.C.7). The emissions for air base space heating computed by AQAM-86 deviated from those computed by AQAM-84 for the same reason, namely a change in emission factors (see Fig. 1).
- 2.3.8 Military and civilian vehicle area sources (II.C.9) and II.C.10). All three models disagree on CO, HC, and NOX emissions for vehicle parking. The reason for this deviation lies in the treatment each accords to hot-soak emissions.

¹The notation I.A. corresponds with that of the source inventory listing.

Poliutant	HC NOX PM	0.040 10.50 5.000	0.040 3.25 8.000	0.040 7.00 30.000	45.00 5.000 1.50 7.500 19.50	0.040 9.00 5.000	0.040 5.00 2.500	50.5		0.090 8.00 2.260	0.034 2.40 1.750	0.085 2.20 0.310		23,000 8800.00 48.000	84 000 1600 00 48 000	84.000 1600.00	0.030 1.58 0.035		0.060 1.13 0.035	0.060 1.13 0.035	0.060 1.05 0.030	0.050 1.05 0.030	
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	Æ		9.0	0.5	10.00	8.50	1.00	1.00	5.00	40.36	1.30	42.14	0.31	160.00	150.00	150.00 160.00	,	0.22	27.0	0.00	0.22	0.00	
Pollutant	KON		9 5	200	1.50	13.80	4.60	11.50	2.30	12.60	7.20	7.20	2.30	6250.00	2810.00	1920.00 1280.00			1.20	0.72	1.12	0.72	
ă	¥		0.130	200	10.000	0.015	0.100	0.100	1.250	0.250	0.120	0.350	0.120	640.000	48.000	128.000 128.000	•	0.480	0.0	000	0.081	0.000	
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Figure 1. Original and Revised Emission Factors for Power-Plant and Space-Heater Furnaces.

Revised Emission Factor

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Original Emission Factor

In the source input data, there is entered a number, NHSOAK, which gives for each air base source, the annual number of hot-soaks totalled over all vehicle classes. At the same time, there is computed in the model a number, SOAK, which gives the evaporative loss per hot-soak for automobiles (vehicle class 1).

In AQAM-76, these quantities are processed by the following code segment to compute the quantity A(IP), the annual emissions of pollutant IP by all vehicle classes IV = 1,...,6:

```
A(IP)=0.0

DO IV=1,6

A(IP)=A(IP)+SPDC(IP)*VM(IV)*EMFC(K,IV,IP)

IF(IOPT.EQ.3) THEN

A(IP)=A(IP)+CSEM(IV,IP)*NCDST(IV)

IF(IV.EQ.1)

(A(IP)=A(IP)+SOAK*NHSOAK

END IF

END DO
```

(For vehicle parking area sources, K=1 and IOPT=3). The effect of this algorithm is to add hot-soak losses into automobile (vehicle class 1) emissions alone, which is a reasonable approximation given the definitions of NHSOAK and SOAK. But, to do so for all pollutant types is not reasonable since hot-soak losses are evaporative hydrocarbons (pollutant 2).

In contrast, in AQAM-84 this code segment had changed to:

```
A(IP)=0.0
DO IV=1,6
   A(IP)+A(IP)+SPDC(IP)*VM(IV)*EMFC(K,IV,IP)
   IF(IOPT.EQ.3) THEN
        A(IP)=A(IP)+CSEM(IV,IP)*NCDST(IV)
        IF(IP.EQ.2)
        A(IP)=A(IP)+SOAK*NHSOAK
   END IF
END DO
```

Now the effect is the reverse of AQAM-76. Hot-soak losses are added into hydrocarbon emissions alone, but now they are included in every vehicle class. This cannot be correct in view of the definitions of NHSOAK and SOAK.

In AQAM-86, the code in question reads as follows:

```
A(IP)=0.0
DO IV=1,6
   A(IP)=A(IP)+SPDC(IP)*VM(IV)*EMFC(K,IV,IP)
   IF(IOPT.EQ3) THEN
        A(IP)=A(IP)+CSEM(IV,IP)*NCDST(IV)
        IF(IP.EQ.2.AND.IV.EQ.1)
        A(IP)=A(IP)+SOAK*NHSOAK
   END IF
END DO
```

Now the effect is to add hot-soak losses into total hydrocarbon emissions only for automobiles.

2.4 Comparison of Short-Term Dispersion Analyses

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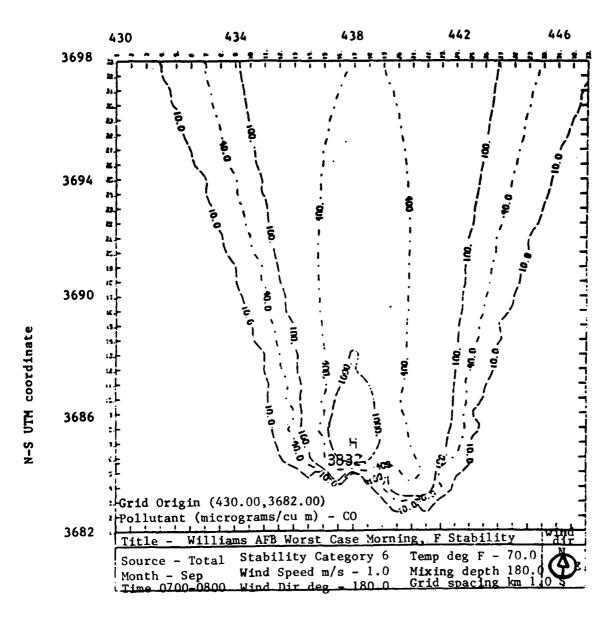
Computer Output C contains short-term dispersion output listings produced by AQAM-76 and AQAM-86 for a specific set of meteorological conditions and source temporal activity fractions. Missing from this document is a similar listing for AQAM-84, since this version of the model gave divide-by-zero errors when it was run. In addition, Figures 2 and 3 show dispersion contour plots (based on the data in Computer Output C) for AQAM-76 and AQAM-86, respectively.

Comparison of the listings in Computer Output C indicates that source emission rates computed by AQAM-86 resemble those computed by AQAM-76. Any differences are attributable to differing annual emission rates computed by the inventory analysis programs (discussed in Sec. 2.3). Note that aircraft source emission rates are difficult to compare because these sources do not carry a unique identification number as do air base and environ sources. (Note also that emission rates are expressed in micrograms per second, a fact which is omitted in the listing in Computer Output C-2 and which will be corrected by USAFOEHL.)

A similar sort of item-by-item agreement is not evident in Computer Output C in the concentration levels computed by the two versions of AQAM. Nevertheless, comparison of Figures 2 and 3 shows that both versions predict a "mountain" of pollution with a steep southern slope and with a ridge extending to the north (to be expected with a wind from the south). In addition, both figures show a southeastern bulge in the mountains which correlates with the southeast end of the flight line. The significant difference in the two contour plots, of course, and in the listings of Computer Output C, is that the mountain predicted by AQAM-76 is "larger" than that predicted by AQAM-86. The peak concentration level in Figure 2 is $3832~\mu g/m^3$; that in Figure 3, $1936.5~\mu g/m^3$. In addition, the 400 and $1000~\mu g/m g^3$ contours in Figure 2 are larger than their counterparts in Figure 3.

A complete explanation for these quantitative differences in pollutant levels predicted by the two models is difficult to generate. Part of the explanation, of course, lies in differing source emission rates; the remainder must be attributed to differences in performing the dispersion computation. With no working model of the AQAM-76 vintage available, resolution of this situation would seem to require the following steps:

- o Generate stand-alone versions of the AQAM-76 and AQAM-86 dispersion modules which allow various source types and geometries, as well as meteorological conditions, to be input to each in a convenient and flexible way.
- o Reconcile the behavior of these two modules to develop a single dispersion module which gives satisfactory performance.
- o Integrate the resulting module into AQAM-86.



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Figure 2. Short Term AQAM Output From Williams Air Force Base 1976 Simulation.

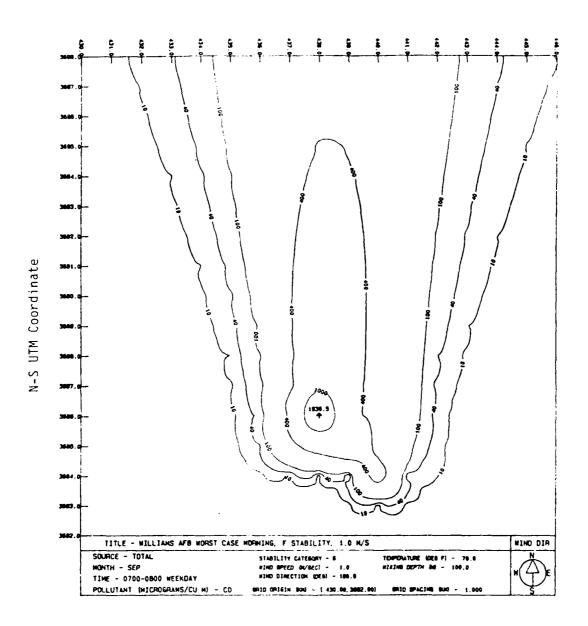


Figure 3. Short Term AQAM Output from Williams Air Force Base 1986 Simulation.

The amount of testing required to accomplish this program made it infeasible for the current effort. The approach for AQAM-86 concentrated on modifying the dispersion module of AQAM-84 as part of the total AQAM system until it appeared to work satisfactorily. The result, described above, is an AQAM dispersion module which runs and which gives results similar to those produced by AQAM-76.

3.0 CONCLUSIONS AND RECOMMENDATIONS

The verification analysis conducted with source data from Williams AFB confirms that the latest version of AQAM residing on the OEHL VAX-11/780 computer is roughly equivalent to the original version of AQAM. With regard to the computation of source emissions, leading to source and emission inventories, the two versions of AQAM differ primarily in the emission factors associated with power-plant and space-heater furnaces. Other notable differences, but minor in comparison, are attributable to changes in the algorighms used to compute GSE emissions, aircraft runway-roll emissions, and ground-vehicle hot-soak emissions.

With regard to the computation of pollutant dispersion levels, the new version of AQAM gives results which are qualitatively close to, and quantitatively within an order of magnitude of, those of the original model. Complete verification of AQAM-86 (i.e., reconciliation of AQAM-86 with AQAM-76) would require an effort beyond the scope of the current one, but one which USAFOEHL may wish to pursue in the future.

Continued upgrade of AQAM depends primarily on the maintenance of the emission factors of the model. Of greatest importance are those factors relating to aircraft, GSE, or vehicle model year. Of lesser importance are those factors relating to training fires, furnaces, storage tanks, etc., since these can be expected to change seldom by comparison.



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